Module 3: Evaluating the Environmental Performance of a Flowsheet

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Module 3: Evaluating the Environmental Performance of a Flowsheet

- Educational goals and topics covered in the module
- Potential uses of modules in chemical engineering courses
- Student handouts
- Instructor materials
- Software
- Case study / Software Demonstrations

Module 3: Educational goals

Students will:

- become aware of potential environmental impacts for releases from chemical processes
- be able to formulate metrics of environmental impact based upon selected chemical properties
- be able to apply the environmental metrics within chemical process design activities using process simulator output
- be aware of the limitations of the environmental assessment framework

Module 3: Topics covered

- Formulating environmental metrics for chemical process designs
- Evaluating chemical process simulator output
  - » Stream and unit summaries ; mass and energy
  - » Air emissions estimation
  - » Environmental fate and transport of emissions and releases
  - » Multiple environmental impact metrics

Module 3: Potential uses of the module in chemical engineering courses

- Design course:
  - » Comprehensive process flowsheet environmental assessment
  - » Compare flowsheet technologies and configurations
  - » Optimize process designs based on environmental impact
- Transport Phenomena course:
  - » Module on interphase mass transfer in the environment

Module 3: Student handouts

- Chapter 11 from textbook: ***Evaluating the Environmental Performance of a Flowsheet***
- Class lecture notes:
  - » edited from chapter 11
  - » instructor writes in key concepts and calculations during the lecture
- Problem 1: Evaluation of Solvent Recycle
  - » Development of environmental metrics
  - » Environmental assessment of a chemical process

Module 3: Instructor materials

- Completed class lecture notes:
  - » edited from chapter 11
  - » contains material that the instructor writes into the notes during the lecture
- Problem 1: Evaluation of Solvent Recycle
- Software for estimating metric properties

Module 3: Emissions estimation software

- Air Chief CD ; EPA 1998
- Tanks4 ; EPA 1999

SOFTWARE DEMONSTRATION

- Emission Master ; Mitchell Scientific 1994
- Environmental Fate and Risk Assessment Tool (EFRAT) ; MTU 1999

Module 3: Fate and transport software

- Single Compartment Models
  - » OPPT Tools (ReachScan, PDM3 - Rivers)
  - » Gaussian Plume Model (Atmosphere)
- Multimedia Compartment Models
  - » Mackay Level III ; 1992

SOFTWARE DEMONSTRATION

  - » CalTOX Level IV ; 1994

Module 3: Index generating software

- EFRAT ; MTU 1999

SOFTWARE DEMONSTRATION

- WAR, TRACI ; EPA

Impacts:

- Impacts for Human and Ecosystem Health:
  - » Inhalation route non-carcinogenic toxicity
  - » Inhalation route carcinogenic toxicity
  - » Ingestion route non-carcinogenic toxicity
  - » Ingestion route carcinogenic toxicity
  - » Ecosystem toxicity
- Impacts for abiotic environmental impacts:
  - » global warming ozone depletion
  - » smog formation acidification

Module 3: Constructing metrics using environmental properties

Exposure Potential

Inherent Impact Parameter

$$\text{Dimensionless Risk Index } (I^*) = \frac{[(\mathrm{EP})(\mathrm{IIP})]_{\mathrm{i}}}{[(\mathrm{EP})(\mathrm{IIP})]_{\mathrm{B}}}$$

Benchmark Compound

Chemical “i”

$$\text{Process Index } (I) = \sum_{i=1}^{N} (I^*) \times (m_i)$$

Process Emission Rate

Module 3: Constructing metrics using environmental properties (cont.)

Dimensionless Risk Index	Eqn. #	I* Equations	Parameter / Software Source(s)
Ingestion Route Toxicity Potential	1	$INGTP_i = \dfrac{C_{i,a}/RfD_i}{C_{Toluene,a}/RfD_{Toluene}}$	***$C_{i,a}$ & $C_{Toluene,a}$*** – Mackay Model, 1992-4; **RfD_i & $RfD_{Toluene}$** – EPA 1994, 1997
Inhalation Route Toxicity Potential	2	$INHTP_i = \dfrac{C_{i,a}/RfC_i}{C_{Toluene,a}/RfC_{Toluene}}$	***$C_{i,a}$ & $C_{Toluene,a}$*** – Mackay Model, 1992-4; **RfC_i & $RfC_{Toluene}$** – EPA 1994, 1997
Ingestion Route Carcinogenicity Potential	3	$INGCP_i = \dfrac{C_{i,w} \times (SF_i)_{ING}}{C_{Benzene,w} \times (SF_{Benzene})_{ING}}$	***$C_{i,w}$ & $C_{Benzene,w}$*** – Mackay Model, 1992-4; ***SF***- EPA 1994, 1997
Inhalation Route Carcinogenicity Potential	4	$INHCP_i = \dfrac{C_{i,a} \times (SF_i)_{INH}}{C_{Benzene,a} \times (SF_{Benzene})_{INH}}$	***$C_{i,w}$ & $C_{Benzene,w}$*** – Mackay Model, 1992-4; ***SF***- EPA 1994, 1997
Fish Toxicity Potential	5	$FTP_i = \dfrac{C_{i,w} \times LC_{50f,PCP}}{C_{PCP,w} \times LC_{50f,i}}$	***$C_{i,w}$ & $C_{PCP,w}$*** – Mackay Model, 1992-4; ***LC_{50f}*** - Verschueren, 1996; Davis, 1994

Module 3: Constructing metrics using environmental Properties (cont.)

Dimensionless Risk Index	Eqn. #	I* Equations	Parameter / Software Source(s)
Global Warming	6	GWP_i	***GWP-*** Fisher, 1990a; WMO, 1992a; IPCC, 1991, 1996
	6a	$GWP_i = N_C \times \frac{MW_{CO_2}}{MW_i}$	***N_C*** –
Ozone Depletion	7	ODP_i	***ODP-*** Fisher, 1990b; WMO, 1990a; WMO 1992b
Smog Formation	8	$SFP_i = \frac{MIR_i}{MIR_{ROG}}$	***MIR-*** Carter, 1994; Heijungs, 1992
Acid Rain	9	ARP_i	***ARP-*** Heijungs, 1992; Goedkoop, 1995

Module 3, Problem 1: Design of a Mixed Solvent Recycle Process

Gaseous waste streams that contain volatile organic compounds (VOCs) are common in industry.

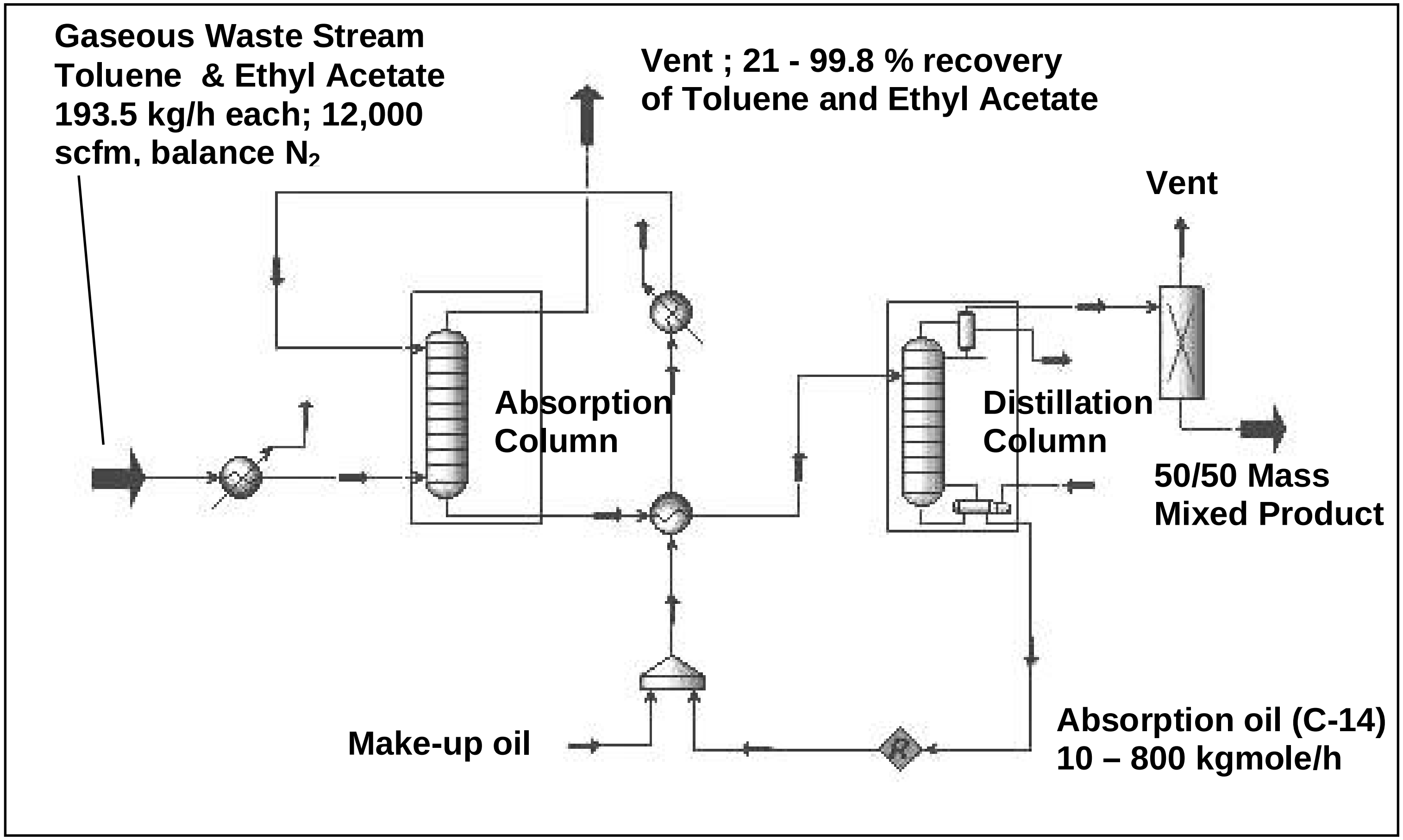
Recovering and recycle of these solvents may increase profitability and reduce environmental impacts.

Environmental impact assessment can help identify optimum VOC recovery.

Module 3, Problem 1: Overview

- Construct flowsheet: Absorption into heavy oil followed by Distillation
- Run process simulator for several heavy oil flow rates
- Estimate emissions / emissions table
- Environmental fate and transport of emissions
- Environmental metrics summary
- Compare flowsheet configurations

Module 3, Problem 1: Flowsheet



Module 3, Problem 1: Emissions Calculations ; 100 kgmole / hr

Energy Related Emissions

$$SOx\ (kg/hr) = \frac{\overbrace{(6.16x10^6\ \text{Btu/hr})}^{\text{Reboiler Duty}}\overbrace{(18\text{kg SOx/1000 L/\%S})}^{\text{Emission Factor}}\overbrace{(1\%\ \text{S})}^{\text{\% Sulfur}}}{\underbrace{(0.70)}_{\text{Bioler Efficiency}}\underbrace{(38.3x10^6\ \text{Btu/1000 L})}_{\text{Fuel Value}}}$$

Unit Operations Emissions : Distillation Column

$$Toluene\ (kg/hr) = \underbrace{(0.75)}_{\text{Mass Fraction Toluene}}\overbrace{(0.1\text{g Toluene/kg flow})}^{\text{Emission Factor}}\overbrace{(258.10\ \text{kg flow/hr})}^{\text{Condenser Flow}}$$

Module 3, Problem 1: Unit Operations-Specific Emissions

UNIT OPERATION	"METHOD"	Mass Flow (kg/hr)	Emission rate (kg/hr)							
			Toluene	Ethyl Acetate	C-14	SOx	NOx	CO_2	CO	TOC
Absorption Column	"HYSIS"	19,840	0.002	128	4.23					
Distillation Column	"emission factor"	259.1	0.019	0.007						
Fugitive Sources	"emission factor"	259.1	0.062	0.062						
Storage Tank	"correlation"	259.1	0.0014	0.0014						
Reboiler Energy (10^6 Btu/hr)		6.16				3.93	0.52	499	0.129	0.007
Total Emissions (kg/hr)			0.088	128.07	4.23	3.93	0.52	499	0.129	0.007

Where are the centers for energy consumption and emissions?

100 kgmole/hr Oil Flow Rate

Module 3, Problem 1: Emissions Summary

Flow rate (kgmole/hr)	Emission rate (kg/hr)							
	Toluene	E.A.	SOx	NOx	CO_2	CO	TOC	n-C14
0	193.55	193.55	0.00	0.00	0.00	0.00	0.00	0.00
10	119.87	185.87	0.41	0.05	51.69	0.01	0.00	4.28
20	53.11	178.37	0.81	0.11	103.26	0.03	0.00	4.83
50	0.97	160.40	1.99	0.26	252.64	0.07	0.00	4.67
100	0.09	128.07	3.93	0.52	498.80	0.13	0.01	4.23
200	0.02	59.95	7.82	1.03	991.29	0.26	0.01	4.13
300	0.02	12.87	11.69	1.54	1482.48	0.38	0.02	4.06
400	0.03	1.70	15.56	2.05	1972.87	0.51	0.03	4.05
500	0.03	0.27	19.42	2.56	2463.25	0.64	0.03	4.04

Module 3, Problem 1: Environmental Fate Summary

Toluene Data	
Molecular weight, g/mol	92.13
Melting point, ˚C	-95
Solubility in Water, g/m^3	550
Vapor pressure, Pa	3800
log Kow	2.7
Degradation half-lives, hr	
- in air compartment	10
- in water compartment	200
- in soil compartment	200
- in sediment compartment	2000

	C_A (g/m^3)	C_W (g/m^3)
Emitted Chemicals		
Toluene	1.26E-07	1.73E-07
Ethyl Acetate	1.26E-07	1.32E-06
n-Hexane	1.26E-07	5.63E-10
Tetradecane	9.88E-08	6.82E-10
Benchmark Chemicals		
Toluene	1.26E-07	1.73E-07
Pentachlorophenol	6.58E-07	1.05E-04

Mackay Level III Multimedia Compartment Model

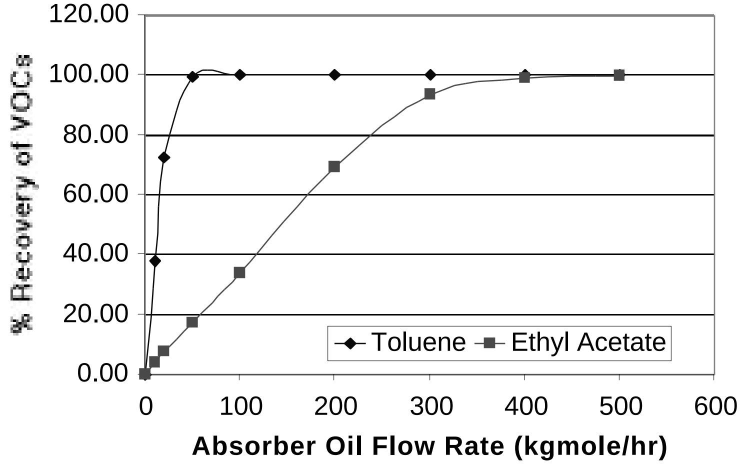
Module 3, Problem 1: Risk Index Summary

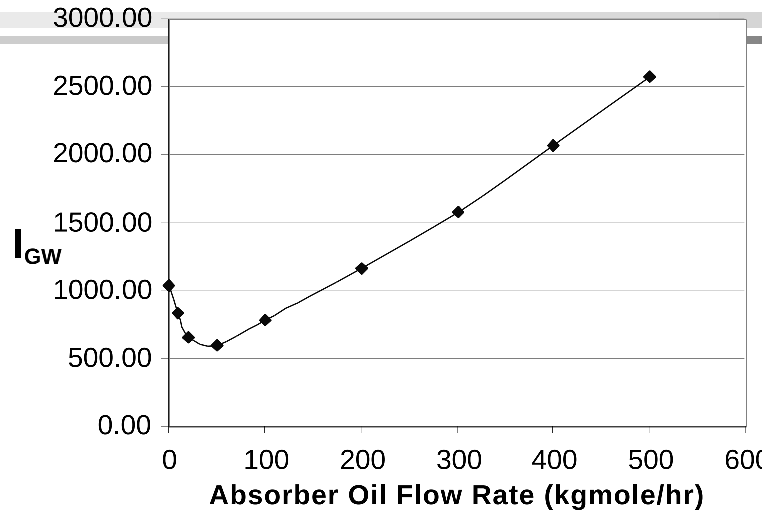
Unitless	Relative Risk Index (I*)								
Compound	GWP	ODP	SFP	ARP	INGTP	INGCP	INHTP	INHCP	FTP
Toluene	3.34	0	4.3	0.0	1	0	1.0	0	0.02
Ethyl Acetate	2	0	0.9	0.0	110	0	0.3	0	0.76
SOx	0	0	0.0	1.0	0	0	0.0	0	0.00
NOx	40	0	0.0	0.7	0	0	0.0	0	0.00
CO2	1	0	0.0	0.0	0	0	0.0	0	0.00
CO	2	0	0.9	0.0	0	0	50.0	0	0.00
C-23	3.1	0	0.0	0.0	0	0	0.0	0	0.00
C-14	3.1	0	0.0	0.0	0	0	0.0	0	0.00
TOC	3.1	0	1.6	0.0	0	0	0.0	0	0.00

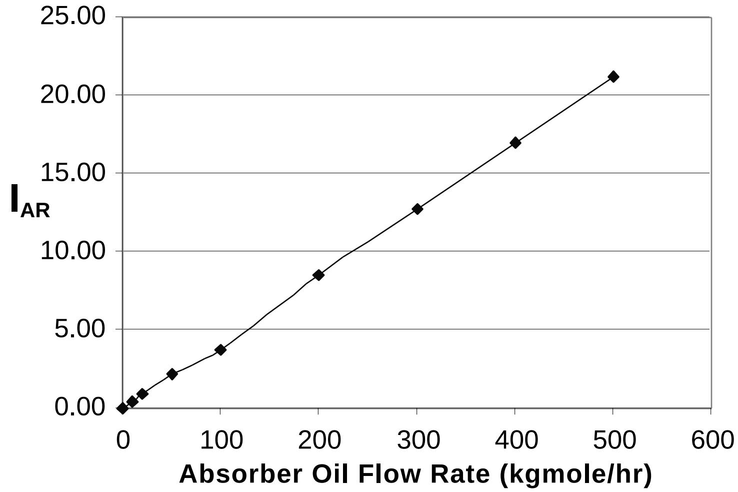
Which chemicals have the highest impact indexes?

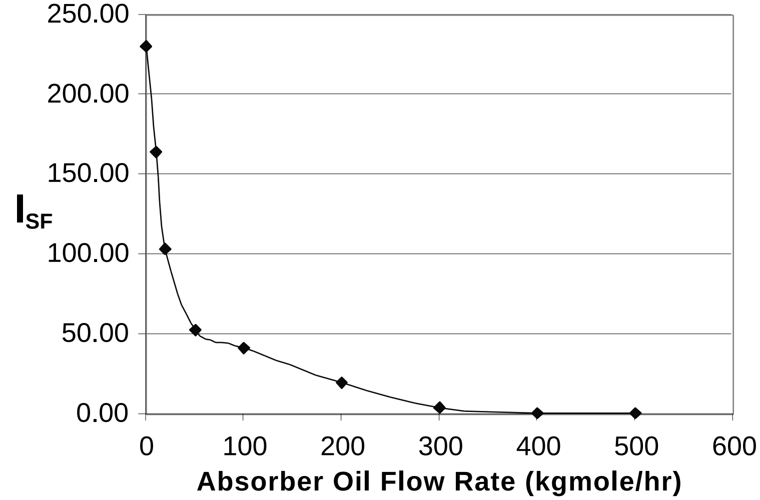
$$\text{Process Index } (I) = \sum_{i=1}^{N} (I_i^*) \times (m_i)$$

Module 3, Problem 1: Comparing Processes Based on Impact









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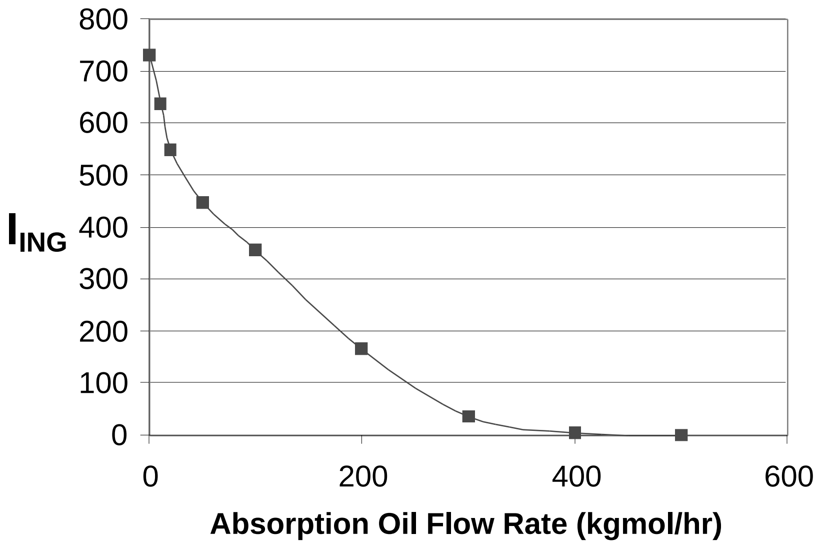

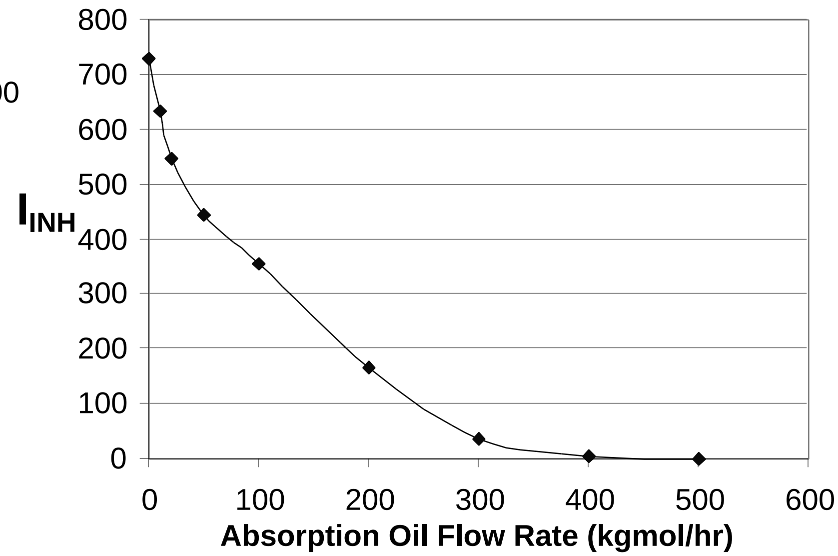

Module 3, Problem 1: Further Inquiry

- Can the process be improved based on environmental impact?
  - » Effects of material choices (absorber oil)
  - » Degree of heat integration in process
  - » Effects of fuel type (reduce SOx)
  - » Optimize reflux ratio on distillation column
  - » Look upstream (substitutes for toluene and ethyl acetate?)

Module 3: Summary of Software Needed

1. COMMERCIAL PROCESS SIMULATOR
   - » mass balances, energy balances, stream data, equipment sizes, air/water releases
2. AIR EMISSIONS ESTIMATION
3. MACKAY ENVIRONMENTAL FATE MODEL
   - » concentrations of released chemicals in air, water, soil, and sediment
   - » Run EPIWIN for properties
4. ENVIRONMENTAL METRICS SOFTWARE